

Temperature dependent Fermi arcs in the normal state of the underdoped cuprate superconductors

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Angle resolved photoemission experiments by Kanigel, et al [Nature Physics 2, 447 (2006)] have made a remarkable observation that low energy electronic excitations in the normal state of underdoped cuprate superconductors exist on open “Fermi arcs” instead of a closed Fermi surface. These arcs shrink upon cooling, with the arc length appearing to extrapolate to nodal points at zero temperature. We show that this striking non-Fermi liquid behavior could result from the underdoped normal state above T_c lying in the vicinity of a quantum phase transition between a d-wave superconductor and a correlated insulating phase.

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Introduction. — The normal state of the underdoped high temperature superconductors (SCs) has long been argued to lie outside the paradigm of Fermi liquid theory due to strong electron correlations. The most remarkable manifestation of this appears in recent angle resolved photoemission spectroscopy (ARPES) studies [1] above the superconducting transition temperature (T_c) in underdoped (UD) $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$. These experiments show that the spectral weight of low energy single particle excitations is not present on a closed Fermi surface (FS) in momentum space. Instead, it forms open “Fermi arcs” [1] of length $\sim T/T^*$, where T^* is the pseudogap temperature, indicating a complete breakdown of the Fermi surface between T_c and T^* . One can envision two very different causes for such NFL behavior.

(i) The ARPES experiments could be probing the finite temperature properties of some exotic non-SC ground state which competes with d-wave superconductivity at low doping. Since the Fermi arcs appear to extrapolate to nodal points enclosing zero volume [1] as $T \rightarrow 0$, this “underlying normal state” must be a non-Fermi liquid as it violates Luttinger’s theorem [2, 3, 4]. Varma and Zhu [5] have postulated a time-reversal symmetry breaking phase with circulating currents and argued that current fluctuations in this phase can lead to Fermi arcs. Other proposals for candidate underlying normal states include the d-density wave [6] and staggered flux phases [7]. With varying doping, these two states support hole pocket Fermi surfaces with an area proportional to the doping, although the spectral weight around this pocket is anisotropic and has been argued to lead to an arc-like feature. Another concern with these two states is that the “arcs” in such models do not appear to extrapolate into nodal points as $T \rightarrow 0$. One more recent proposal for arcs involves inducing an additional nematic liquid crystalline order in the SC state at low doping [8] but so far it has not addressed the normal state above T_c .

(ii) A second possibility is to examine whether order parameter fluctuations of the d-wave SC or fluctuations of the short range antiferromagnetic order above T_c could

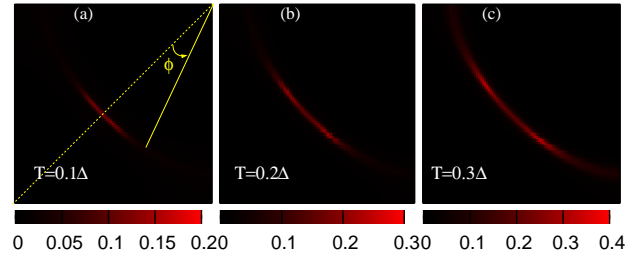


FIG. 1: (color online) Temperature evolution of Fermi arcs, regions of significant $A(\mathbf{k}, \omega = 0)$ in the first quadrant of the Brillouin zone.

lead to Fermi arc physics. This has been examined earlier using various approaches [9], although these works have not focussed on the temperature scaling of the arc length. A distinct way to study thermal order parameter fluctuations is to consider the effect of a dilute gas of classical vortices [10] above T_c . Alternatively, at low dopings and temperatures, quantum fluctuations of the order parameter are also relevant; such quantum fluctuations could be particularly important if one is close to a quantum phase transition out of the superconducting state into a correlated insulating state.

In this paper we will explore this last route. Namely, we study the possibility that the Fermi arcs in the underdoped normal state arise from proximity to a quantum phase transition between a d-wave SC and a correlated insulating state at low doping. Fig. 1 illustrates one of the key results of this paper — the computed zero energy spectral function for the model which we study in this paper shows temperature dependent Fermi arcs in the normal state as seen in ARPES.

There are several experimental motivations to explore this route which we follow. First, the observed gap structure in the normal state appears to extrapolate smoothly with lowering temperature to a SC gap with a pure d-wave form over a range of dopings. This suggests that any “underlying normal state” scenario has to be specifically chosen to extrapolate into the excitation spectrum of the d-wave state over a whole range of dopings. This seems,

to us, to be slightly unnatural although we cannot rule it out. It appears more natural to assume that the normal state has fluctuating d-wave correlations. Second, the arc length seen in the experiments appears to scale linearly with temperature and independent of most microscopic details. Such a simple T -dependence suggests proximity to a quantum phase transition near which the temperature naturally arises as the only energy scale. Finally, NFL behavior has been observed in a variety of other materials [11, 12] near field or pressure tuned quantum phase transitions. Given this ubiquity of NFL behavior in the vicinity of quantum phase transitions, it is worth examining this scenario also for the underdoped cuprates. Our proposal receives support from penetration depth measurements [13] on $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ which appear to be probing the low temperature manifestations of a 3D SC-insulator quantum phase transition [14, 15]. Recent tunneling experiments [16] in other cuprates also show that the SC state at low hole density is destroyed by charge localization leading to such a SC-insulator transition.

SC-insulator transition, critical charge fluctuations and the electron spectral function. — The underdoped cuprate SCs are doped correlated insulators, and the strongly correlated Hubbard model is thought to be a possible minimal description of this system [17]. At large U , this leads to an effective tJ model with a kinetic energy for the doped holes and a superexchange interaction between the spins. In order to calculate the electron spectral function in such a system, we appeal to slave-boson mean field theory [17, 18, 19, 20] which decomposes the electron operator into a product of a spin-1/2 neutral spinon and a spinless charge-1 boson, $c_\sigma^\dagger(\mathbf{r}, \tau) \sim f_\sigma^\dagger(\mathbf{r}, \tau)\Psi(\mathbf{r}, \tau)$. These two particles are coupled by gauge fields enforcing the non-double occupancy constraint. At mean field level [17, 18], the spinons and charges are decoupled since gauge fluctuations are ignored — the SC state then corresponds to d-wave pairing of spinons and condensation of the bosons. Despite this drastic approximation, the SC correlations obtained in this theory are in remarkable qualitative agreement with a careful treatment using Gutzwiller projected wavefunctions. This wavefunction approach works directly with electronic degrees of freedom, and has been shown to *quantitatively* explain a variety of photoemission and optical conductivity data [21] in the SC state. At finite temperature, gauge fluctuations around the mean field state are more important; however their effect has been shown to be mitigated in the presence of critical boson fluctuations [22] (which we are interested in here), although the gauge fluctuation corrections to the results presented here remains an important problem for future work. For now, we will therefore view slave boson mean field theory as a crude but qualitatively reasonable way to proceed, in order to see what aspects of the phenomenology of the underdoped cuprates can be possibly captured.

With underdoping, the SC undergoes a quantum phase

transition into a correlated insulating state which, as suggested by tunneling experiments [16], has glassy bond-centered charge order which could arise from the Coulomb interactions between the bosons. However, in order to expose the physics of the Fermi arcs we choose to study a simpler model of a SC-insulator transition, where the boson field $\Psi(\mathbf{r}, \tau)$ is described by a Ginzburg Landau action

$$S_\Psi = \int d\tau d^3\mathbf{r} \left(|\partial_\tau \Psi|^2 + c^2 |\nabla \Psi|^2 + m^2 |\Psi|^2 + \frac{g}{2} |\Psi|^4 \right). \quad (1)$$

Note the SC is three-dimensional and anisotropic, $c^2 |\nabla \Psi|^2$ is the short hand notation for $c_\parallel^2 |\nabla_\parallel \Psi|^2 + c_z^2 |\partial_z \Psi|^2$, with $c_z \ll c_\parallel$. For $m^2 > 0$, the system is in a uniform insulating phase with a charge gap. For $m^2 < 0$, the SC state with a nonzero $\langle \Psi \rangle$ is more stable. The mean field SC-insulator critical point is at $m^2 = 0$. Model (1) is at its upper critical dimension and we can drop the quartic interaction at $T = 0$. The critical boson Green function is then $\chi(\mathbf{Q}, i\nu_n) = \langle \Psi_{\mathbf{Q}, i\nu_n}^* \Psi_{\mathbf{Q}, i\nu_n} \rangle = 1/(\nu_n^2 + \Omega_{\mathbf{Q}}^2)$, where $\mathbf{Q} \equiv (\mathbf{q}, q_z)$ is the 3D momentum with \mathbf{q} being its ab-plane component, $\Omega_{\mathbf{Q}}^2 = c_\parallel^2 \mathbf{q}^2 + c_z^2 q_z^2$, and $\nu_n = 2n\pi T$. Sitting at $m^2 = 0$ and warming up from zero temperature, the quartic interaction induces [23] a T -dependent mass R leading to the charge fluctuation propagator

$$\chi^{-1}(\mathbf{Q}, i\nu_n) = \nu_n^2 + \Omega_{\mathbf{Q}}^2 + R \quad (2)$$

Leading order perturbation theory in g at 1-loop (Hartree) level yields $R = 4g \sum_{\mathbf{Q}} \Omega_{\mathbf{Q}}^{-1} n(\Omega_{\mathbf{Q}})$, where $n(x) = 1/(e^{x/T} - 1)$ is the Bose function. At finite temperature, the interaction also induces a damping term in the boson Green function. This thermal relaxation rate is however higher order in g in a perturbative treatment, and we ignore it here. A description of the thermal relaxation rate over a range of energies from small to large values of ν/T is nontrivial [23]; we have so far not pursued this calculation.

We assume the spinons are paired in the d-wave channel throughout the transition, and described by a d-wave Bardeen-Cooper-Schrieffer type Hamiltonian with a kinetic energy $\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$, and a d-wave pairing gap $\Delta_{\mathbf{k}} = \Delta(\cos k_x - \cos k_y)/2$, with the resulting quasiparticle dispersion $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$. Support for this approximation comes from thermal transport measurements [24] which indicate that the thermal conductivity, which is dominated by nodal d-wave quasiparticles in the SC state, *remains unchanged when we enter the non-superconducting state below a critical doping*. Using this, the electron Green function can be obtained by convolving its spinon and boson parts,

$$G(\mathbf{k}, ik_n) = \sum_{\mathbf{Q}} \frac{F_1 u_{\mathbf{k}-\mathbf{Q}}^2 + F_2 v_{\mathbf{k}-\mathbf{Q}}^2}{2N\omega_{\mathbf{Q}}}. \quad (3)$$

where N is the number of sites,

$$F_1 = \frac{1 + n(\omega_{\mathbf{Q}}) - f(E_{\mathbf{k}-\mathbf{q}})}{ik_n - E_{\mathbf{k}-\mathbf{q}} - \omega_{\mathbf{Q}}} + \frac{n(\omega_{\mathbf{Q}}) + f(E_{\mathbf{k}-\mathbf{q}})}{ik_n - E_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{Q}}},$$

$$F_2 = \frac{1 + n(\omega_{\mathbf{Q}}) - f(E_{\mathbf{k}-\mathbf{q}})}{ik_n + E_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{Q}}} + \frac{n(\omega_{\mathbf{Q}}) + f(E_{\mathbf{k}-\mathbf{q}})}{ik_n + E_{\mathbf{k}-\mathbf{q}} - \omega_{\mathbf{Q}}}.$$

Here $\omega_{\mathbf{Q}} = \sqrt{\Omega_{\mathbf{Q}}^2 + R}$, $f(x) = 1/(e^{x/T} + 1)$ is the Fermi function, and $u_{\mathbf{k}}^2 = (1 + \xi_{\mathbf{k}}/E_{\mathbf{k}})/2$ and $v_{\mathbf{k}}^2 = 1 - u_{\mathbf{k}}^2$ are the usual BCS coherence factors. Our work is quite close in spirit to the zero temperature calculations of Ref. [25].

After analytic continuation, $ik_n \rightarrow \omega + i0^+$, the imaginary part of Eq. (3) gives the electron spectral function $A(\mathbf{k}, \omega)$. The result is easy to understand qualitatively. An electron with energy ω and in-plane momentum \mathbf{k} is made by combining a spinon and a boson. However, the spinon Green function has weight at energies $\pm E_{\mathbf{k}-\mathbf{q}}$ and the boson excitations also has weight at $\pm \Omega_{\mathbf{Q}}$ (as seen from the boson Green function in Eq. 2) which leads to four contributions to the electron spectral function. The thermal and coherence factors appearing in the spectral function appropriately weight the probability of such processes.

Fermi arcs in $A(\mathbf{k}, 0)$. — We first argue that Eq. (3) leads to Fermi arcs centered around the nodes of the d-wave SC dispersion if we focus on the zero energy spectral function $A(\mathbf{k}, 0)$. In order to make the qualitative argument, let us work at very low temperatures such that $T \ll \Delta, c_{\parallel}\Lambda, c_{\perp}\Lambda$. In this low temperature regime, the interaction induced mass $R \sim T^2$. Thus, the characteristic boson fluctuations will have very small in-plane momenta $|\mathbf{q}| \sim (T/c_{\parallel}) \ll \Lambda$, small overall momentum $|\mathbf{Q}| \ll \Lambda$, and energies $\sim T$. In order to obtain a zero energy electron with a certain momentum \mathbf{k} , we have to use the energy of this thermal boson fluctuation to excite a spinon quasiparticle, namely spinon quasiparticles with binding energy $\sim T$. The zero energy electron will have nearly the same in-plane momentum as the spinon quasiparticle (since the boson carries very little momentum). Given these constraints, and the fact that spinon quasiparticles with energy $\sim T$ lie on banana shaped arcs of size $\sim T/\Delta$ around the d-wave nodes of the SC, it is clear that the zero energy electrons will also lie on “Fermi arcs” of size T/Δ around the nodes of the underlying d-wave SC. Since $T^* \sim \Delta$ in the cuprates, this is consistent with (T/T^*) scaling of Fermi arcs reported in Ref. [1].

The above rough argument relied on working at very low temperature. We next proceed to a numerical evaluation of the electron spectral function $A(\mathbf{k}, 0)$ in order to justify this argument and also to study the evolution upto temperatures $T \sim \Delta$. We have numerically evaluated $A(\mathbf{k}, 0)$ using Eq.(3) for temperatures of interest to the ARPES experiments ($T = 0.1\Delta - 0.9\Delta$). We work at doping $\delta = 0.05$ and choose $t'/t = -0.25$, $\Delta/t = 0.15$ for the spinons. Also we set $c_{\parallel}\Lambda = 3t \gg \Delta$, $c_z = c_{\parallel}/300$, and use a Lorentzian broadening of $0.01t$ in Eq.(3). The

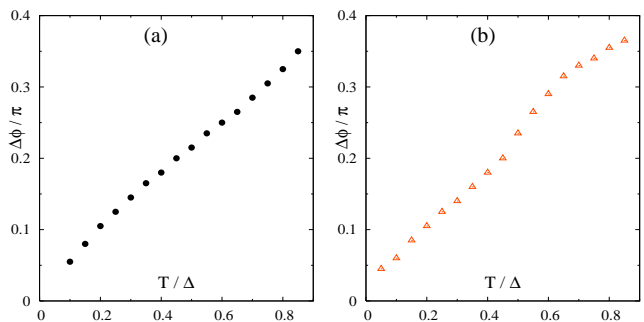


FIG. 2: (color online) Estimate for the arc length $\Delta\phi$ from the zero energy spectral weight $A(\phi, 0)$ for angles ϕ along the FS (defined in Fig. 1). (a) Arc length defined as angular distance between points of maximum $A(\phi, 0)$ along the Fermi surface. (b) Arc length defined as the region with half the total spectral weight along the FS. See text for details.

results for $g = 0.1$ are plotted in Fig. 1 for $0 < k_x, k_y < \pi$, qualitatively similar results are found for other values of g . We see from Fig.1(a-c) that $A(\mathbf{k}, 0)$ forms open arcs in momentum space with negligible (although nonzero) weight at other momenta on the Fermi surface.

Size of the Fermi arcs. — In order to measure the size of the Fermi arcs, we analyze the zero energy momentum distribution curve along the spinon Fermi surface, $A(\phi, 0)$, where ϕ is the angle from the $(0,0)$ - (π, π) diagonal as shown in Fig.1(a). Going from the nodal towards the antinodal direction along the spinon Fermi surface, $A(\phi, 0)$ first reaches its peak value at ϕ_{max} and then drops to a minimum (background) value of A_{bg} at $\phi = \pi/4$. We use $\Delta\phi = 2\phi_{max}$, i.e. the angular span between two spectral peaks along the Fermi surface, as a first measure of the arc size. Its approximately linear T -dependence is shown in Fig. 2(a).

An alternative measure for the arc size is given by $\Delta\phi = 2\phi_h$, where the region $0 < \phi < \phi_h$ accounts for half the total integrated spectral weight, $\int_0^{\phi_h} d\phi [A(\phi, 0) - A_{bg}] = \frac{1}{2} \int_0^{\pi/4} d\phi [A(\phi, 0) - A_{bg}]$. $\Delta\phi$ defined in this way is shown in Fig. 2(b). We see that both definitions yield the similar qualitative result that $\Delta\phi$ scales linearly with T . This is consistent with our earlier arguments. (The quantitative agreement between the two definitions above is sensitive to the details of what percentage of the spectral weight is chosen in the second definition.)

While the above two definitions of the arc length are accessible theoretically, they are harder to measure in experiments due, atleast, to momentum dependent matrix elements. We therefore turn to results for the EDC at fixed momentum.

Energy distribution curve (EDC) lineshape. — Fig. 3 shows the EDC, namely $A(\phi, \omega)$, plotted over a range of temperatures and angles along the Fermi surface. At all angles, we find that there is a filling-in of low energy spectral weight as the temperature is raised. In our model, this spectral weight growth is facilitated by the tempera-

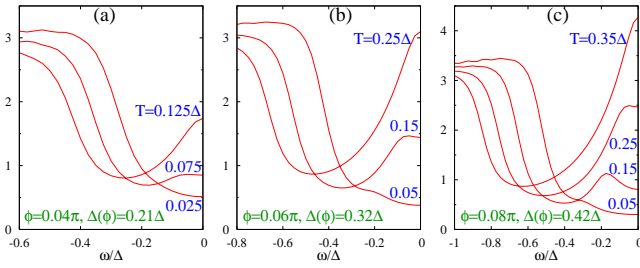


FIG. 3: (color online) Energy distribution curve $A(\phi, \omega)$ for various angles ϕ along the FS, and for increasing temperature showing the filling in of the low energy spectral weight. For angles closer to the node as in (a), the filling in of the spectral weight occurs at lower temperatures consistent with experiments. See text for discussion.

ture dependent mass R which transfers weight from high to low energies. The recovery of zero energy spectral weight occurs at lower temperature for near-nodal points (smaller ϕ) than at angles closer to the antinodal direction. This growth of the low energy spectral weight is such that the dip-like EDC at low energy evolves into a peak-like structure which at sufficiently high temperature becomes a dominant feature.

The above results are broadly consistent with the experimental observations [1]. While the detailed EDC lineshape is not quite like the experimental lineshape, the comparison is expected to improve if we take into account the following points which have been ignored in our analysis. (i) The shift of the higher energy edge-like feature to larger ω could be somewhat offset by a temperature-dependent spinon pairing gap as the local singlet correlations weaken with increasing T — this needs a more careful self-consistent calculation of the spinon gap. (ii) The low energy lineshape may improve if relaxational dynamics for the bosons [23] is taken into account. (iii) Our model Eq.(3) also ceases to be a good approximation at large energies where other inelastic channels, including spin fluctuations, become important. (iv) The nonzero energy resolution of the ARPES experiments ($\sim 15 - 30 \text{ meV}$) has not been taken into account here. Given these limitations, we have not attempted a more detailed analysis to extract the arc length from the EDC as in the experiments.

Discussion. — We have explicitly shown, within a phenomenological slave-boson approach, that critical charge fluctuations near a SC-insulator transition as described by Eq. (1), together with spinon pairing in the d-wave channel, gives rise to Fermi arcs with size $\sim T/T^*$. We finally present some arguments for how the normal state of weakly doped cuprates probed in ARPES experiments [1] could lie in the quantum critical regime of such a transition. Recent tunneling experiments [16] in the weakly doped cuprates indicate that the SC state at low doping undergoes a charge localization into an insulating state. Such a charge localization transition, where the doped

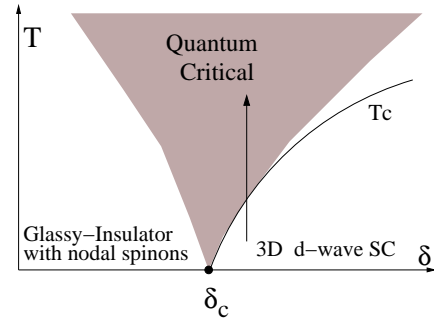


FIG. 4: (color online) Tunneling and thermal conductivity measurements suggest that the cuprate SCs evolve, with doping, from a glassy charge insulator with nodal spinon excitations into a 3D d-wave SC. In the weakly doped regime above T_c , we expect quantum charge fluctuations and Fermi arcs similar to that in the simple model studied here.

holes become immobile, is consistent with a SC-insulator between a d-wave SC and an insulating state which retains d-wave paired spinons. Some hints for the existence of d-wave nodal spinons at low temperature comes from thermal conductivity measurements [24] in samples with $T_c = 0$, which show a residual κ/T very close to that of the SC state at higher doping. This scenario for the SC-insulator transition is sketched in Fig. 4. Warming up above T_c in the low doping regime could thus land us in the quantum critical regime of a SC-insulator transition. Although we have not specifically studied this transition from the SC to a glassy charge-localized insulator with d-wave spinons, we believe our results strongly suggest that this mechanism of critical charge fluctuations near a SC-insulator transition could lead to T -linear Fermi arcs in the underdoped normal state above T_c . It would be interesting to look for more direct experimental signatures of such quantum fluctuations in the underdoped normal state.

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